Angle-Dependent Soft X-Ray Emission Spectra of Hexagonal Boron Nitride

Y. Muramatsu[1] and R. C. C. Perera[2]
[1]*Japan Atomic Energy Research Institute, Sayo-gun, Hyogo 679-5148, Japan*
[2]*CXRO, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA*

Hexagonal boron nitride (*h*-BN) is a basic boron compound, which has been widely used as a reference sample in soft x-ray spectroscopy. It adopts a layered structure similar to graphite. To obtain detailed structural information for *h*-BN using soft x-ray emission spectroscopy, we have measured its angle-dependent soft x-ray emission spectra.

Commercially obtained *h*-BN power pressed on indium sheets and pyrolytic (*p*) BN plate was used for spectroscopic measurements. Soft x-ray emission spectra in the B *K* and N *K* regions were measured using a grating x-ray spectrometer installed in the undulator beamline, BL-8.0.1. The photon energy of the monochromatized incident beam was tuned to about 230 eV (for B *K*) and 430 eV (for N *K*). The incident angle (θ) of the monochromatized beam to the sample surface was adjusted to 15, 45 and 75 degrees. Measured x-ray emission spectra were analyzed using discrete variational (DV)-Xα molecular orbital calculations.

Figure 1 shows the angle-dependent B *K* and N *K* x-ray emission spectra of *p*-BN. In the B *K* spectra, intensity of the high-energy shoulder near 184 eV increases as θ increases. Intensities of the low-energy satellite near 170 eV and the low-energy shoulder near 178 eV both decrease as θ increases. In the N *K* spectra, intensity of the high-energy peak at 398.5 eV drastically increases as θ increases, while intensity of the low-energy shoulders near 385 eV and 390 eV decrease as θ increases. Upper panels of Figure 2 show the calculated density-of-states (DOS) spectra of occupied B2p- and N2p-orbitals in the model cluster of $B_{48}N_{48}H_{24}$. These calculated DOS spectra reproduce the x-ray emission spectra measured with an incident angle of 45 degrees. Lower panels of Figure 2 show the B2p- and N2p-DOS spectra calculated by considering the contributions of σ- and π-components in x-ray emission. In the B2p-DOS spectra, intensity of the high-energy shoulder (near -4 eV) increases as θ increases. Intensities of the low-energy shoulder (-10 eV) and low-energy peak (-18 eV) decrease as θ increases. In the N2p-DOS spectra, intensity of the high-energy peak (-2 eV) increases as θ increases, while intensities of the low-energy shoulders (-6 eV and –10 eV) decrease as θ increases. These calculated spectra well reproduce the measured angle-dependent x-ray emission spectra. Thus, it can be confirmed that angle-dependent x-ray emission measurements will provide detailed structural information on *h*-BN.

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Principal Investigator: Yasuji Muramatsu, Japan Atomic Energy Research Institute. Email: murama@spring8.or.jp. Telephone: +81-791-58-2601.

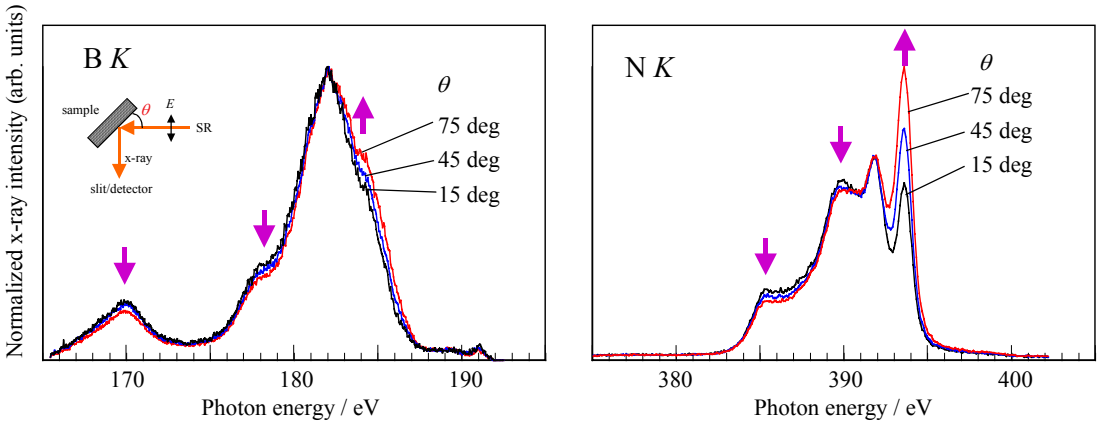

Figure 1 Angle-dependent x-ray emission spectra in the B *K* (left panel) and N *K* (right panel) regions of *p*-BN.

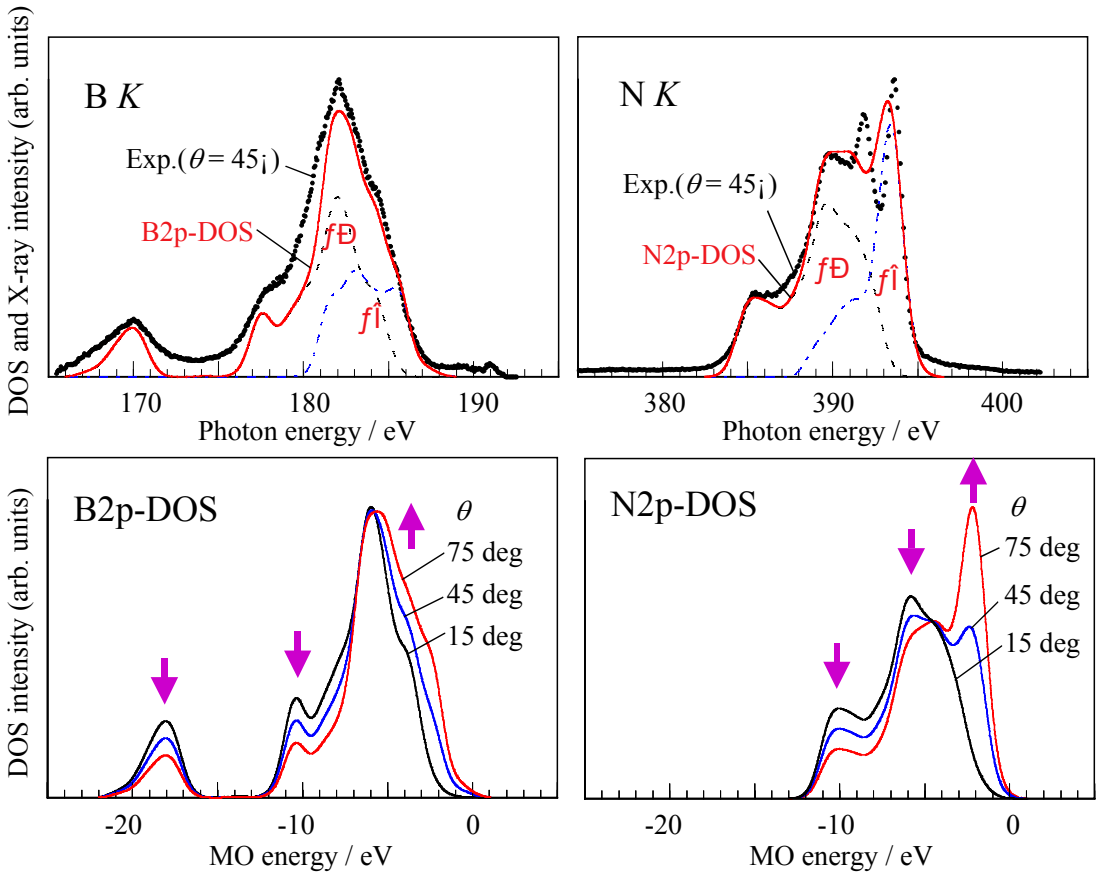

Figure 2 Upper panels show the occupied B2p- and N2p-DOS spectra of the $B_{48}N_{48}H_{24}$ model cluster. X-ray emission spectra measured with an incident angle of 45 degrees are superimposed on the calculated spectra. Lower panels show the angle-dependent B2p- and N2p-DOS spectra with incident angles of 15, 45 and 75 degrees.